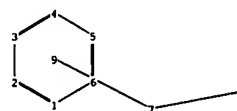
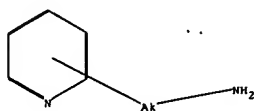


## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1334	((546/290) or (546/334)).CCLS.	US-PGPUB; USPAT	OR	OFF	2007/07/06 10:44
L2	670	1 and amino and methyl and pyridine	US-PGPUB; USPAT	OR	OFF	2007/07/06 11:05
L3	0	("(vangelistiadjmanuel.inv.)").PN.	US-PGPUB	OR	OFF	2007/07/06 11:05



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

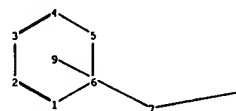
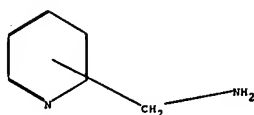
containing 1 :

Connectivity :

7:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

7-8

normalized bonds :

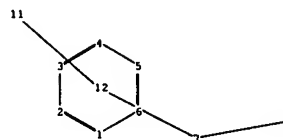
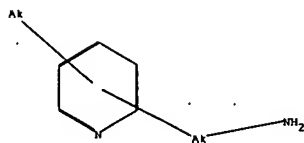
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom



chain nodes :

7 8 11

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

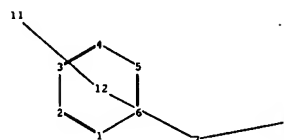
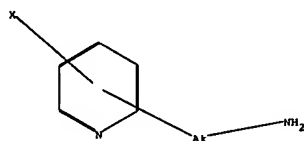
Connectivity :

7:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom

11:CLASS 12:Atom



chain nodes :

7 8 11

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

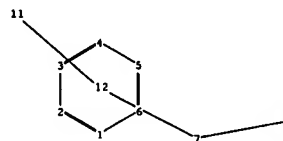
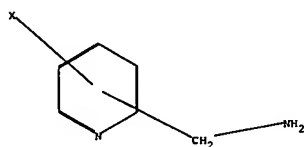
containing 1 :

Connectivity :

7:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom  
11:CLASS 12:Atom



chain nodes :

7 8 11

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

7-8

normalized bonds :

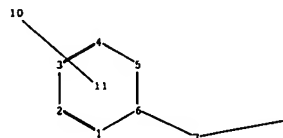
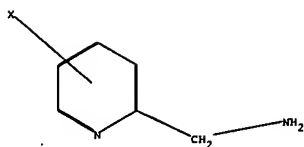
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom  
11:CLASS 12:Atom



chain nodes :

7 8 10

ring nodes :

1 2 3 4 5 6

chain bonds :

6-7 7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

6-7 7-8

normalized bonds :

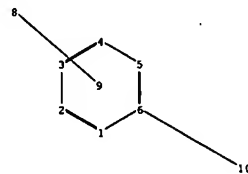
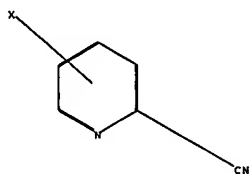
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS  
11:Atom



chain nodes :

8 10

ring nodes :

1 2 3 4 5 6

chain bonds :

6-10

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

6-10

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

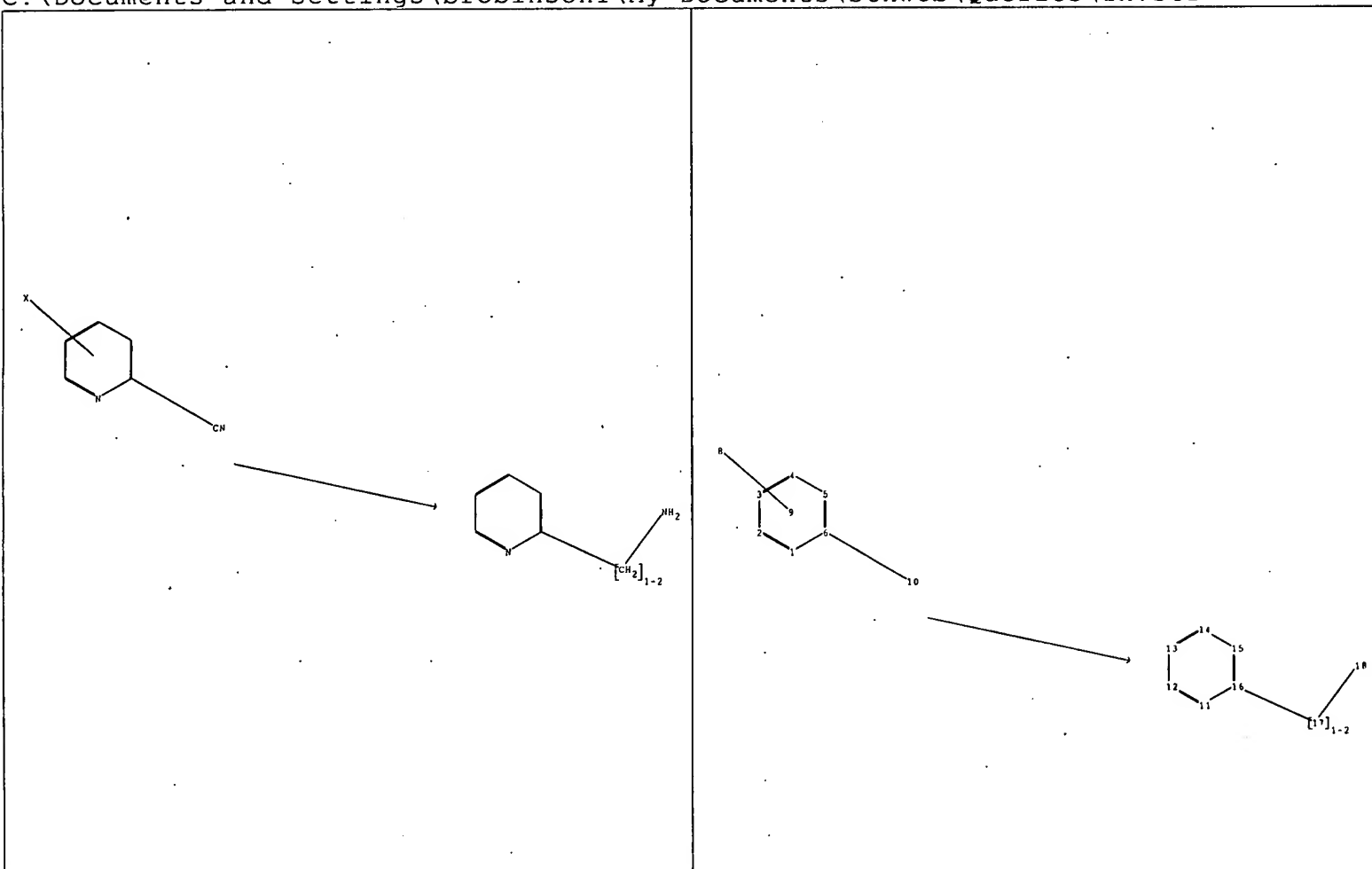
isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:CLASS





chain nodes :

8 10 17 18

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16

chain bonds :

6-10 16-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

exact bonds :

6-10 16-17 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

isolated ring systems :

containing 1 : 11 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:CLASS  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

fragments assigned reactant role:

containing 1

fragments assigned product role:

containing 11

10535723

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal612bxr

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 3 MAR 16 CASREACT coverage extended  
NEWS 4 MAR 20 MARPAT now updated daily  
NEWS 5 MAR 22 LWPI reloaded  
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field  
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 10 APR 30 CA/CAPplus enhanced with 1870-1889 U.S. patent records  
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 12 MAY 01 New CAS web site launched  
NEWS 13 MAY 08 CA/CAPplus Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 17 MAY 21 CA/CAPplus enhanced with additional kind codes for German patents  
NEWS 18 MAY 22 CA/CAPplus enhanced with IPC reclassification in Japanese patents  
NEWS 19 JUN 27 CA/CAPplus enhanced with pre-1967 CAS Registry Numbers  
NEWS 20 JUN 29 STN Viewer now available  
NEWS 21 JUN 29 STN Express, Version 8.2, now available  
NEWS 22 JUL 02 LEMBASE coverage updated  
NEWS 23 JUL 02 LMEDLINE coverage updated  
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names  
NEWS 25 JUL 02 CHEMCATS accession numbers revised  
NEWS 26 JUL 02 CA/CAPplus enhanced with utility model patents from China  
  
NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 4 MAY 2007.  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007

=>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

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=>

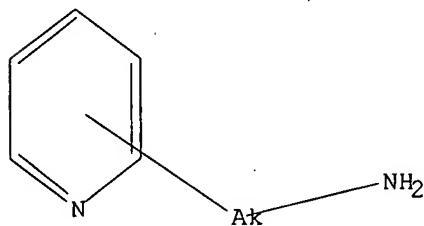
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\2a323f.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Updated Search

10535723

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:14:24 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS 7 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 9162 TO 11916

L2 7 SEA SSS SAM L1

=>

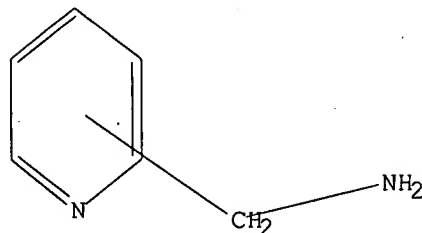
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\rererh.str

L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l3

SAMPLE SEARCH INITIATED 11:15:10 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS 6 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 7759 TO 10309

L4 6 SEA SSS SAM L3

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\qwj.str

Updated Search

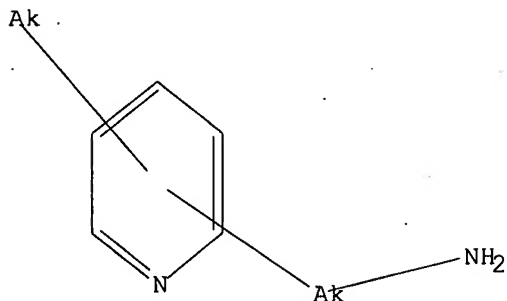
10535723

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 11:16:58 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 4981 TO 7063

L6 4 SEA SSS SAM L5

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\erern.str

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 11:17:38 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

Updated Search

10535723 .

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\qmh.str

L9           STRUCTURE UPLOADED

=> s 19

SAMPLE SEARCH INITIATED 11:18:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -   150568 TO ITERATE

1.3% PROCESSED           2000 ITERATIONS                           0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   \*\*INCOMPLETE\*\*  
                          BATCH    \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS:       2988464 TO   3034256  
PROJECTED ANSWERS:           0 TO           0

L10           0 SEA SSS SAM L9

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\rmgy.str

L11           STRUCTURE UPLOADED

=> s 111

SAMPLE SEARCH INITIATED 11:19:11 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -       9663 TO ITERATE

20.7% PROCESSED           2000 ITERATIONS                           2 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   \*\*COMPLETE\*\*  
                          BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:       187369 TO   199151  
PROJECTED ANSWERS:           7 TO       379

L12           2 SEA SSS SAM L11

=> s 111 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 11:19:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -   192512 TO ITERATE

100.0% PROCESSED   192512 ITERATIONS                           66 ANSWERS  
SEARCH TIME: 00.00.01

L13           66 SEA SSS FUL L11

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
176.60	176.81

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

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FILE COVERS 1907 - 6 Jul 2007 VOL 147 ISS 3  
FILE LAST UPDATED: 5 Jul 2007 (20070705/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 113

L14 89 L13

=> s 1113/prep

L113 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> s 113/prep

89 L13

4427949 PREP/RL

L15

57 L13/PREP

(L13 (L) PREP/RL)

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

2.60

179.41

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=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\oki7.str

L16        STRUCTURE UPLOADED

=> s l16

SAMPLE SEARCH INITIATED 11:20:38 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -        950 TO ITERATE

100.0% PROCESSED        950 ITERATIONS                    13 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                                      BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:        17151 TO        20849  
PROJECTED ANSWERS:            44 TO        476

L17        13 SEA SSS SAM L16

=> s l16 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 11:20:43 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED -        17958 TO ITERATE

100.0% PROCESSED        17958 ITERATIONS                    338 ANSWERS  
SEARCH TIME: 00.00.01

L18        338 SEA SSS FUL L16

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	351.96

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007  
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=> s l18/rct

560 L18  
2989518 RCT/RL  
L19 455 L18/RCT  
(L18 (L) RCT/RL)

=> d his

(FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007)

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

L1 STRUCTURE UPLOADED  
L2 7 S L1  
L3 STRUCTURE UPLOADED  
L4 6 S L3  
L5 STRUCTURE UPLOADED  
L6 4 S L5  
L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 STRUCTURE UPLOADED  
L10 0 S L9  
L11 STRUCTURE UPLOADED  
L12 2 S L11  
L13 66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

L14 89 S L13  
L15 57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

L16 STRUCTURE UPLOADED  
L17 13 S L16  
L18 338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

L19 455 S L18/RCT

=> s l19 and l15

L20 36 L19 AND L15

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

2.60

354.56

FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e nickel/rn

E1 1 99999-98-1/RN  
E2 1 99999-99-2/RN  
E3 0 --> NICKEL/RN

\*\*\*\* END OF FIELD \*\*\*\*

=> e nickel/cn

E1 1 NICKASE TRAA (PLASMID PLW1071) GENE TRAA)/CN  
E2 1 NICKASE-HELICASE (PLASMID TI PLASMID PTI15955 GENE TRAA)/CN  
E3 1 --> NICKEL/CN  
E4 1 NICKEL (0), BIS(METHANETRICARBONITRILATO)DINITROSYLBIS(TRICY  
CLOHEXYLPHOSPHINE)DI-/CN  
E5 1 NICKEL (1+) ACETYLACETONATE/CN  
E6 1 NICKEL (1+), HYDROTRIS(TRIETHYLPHOSPHINE)-/CN  
E7 1 NICKEL (19.2-31.0), ZINC (69.0-80.8) (ATOMIC)/CN  
E8 1 NICKEL (2+) ORTHOPHOSPHATE OCTAHYDRATE/CN  
E9 1 NICKEL (2+), HEXAAMMINE-, BIS(METABORATE)/CN  
E10 1 NICKEL (25.6), TIN (1.5), ZINC (72.9) (ATOMIC)/CN  
E11 1 NICKEL (58Ni1+)/CN  
E12 1 NICKEL (ADENINE) DIBROMIDE/CN

=> s e3

L21 1 NICKEL/CN

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.40	359.96

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007  
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FILE COVERS 1907 - 6 Jul 2007 VOL 147 ISS 3  
FILE LAST UPDATED: 5 Jul 2007 (20070705/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l21

L22 342935 L21

=> s l21/cat

342935 L21

631560 CAT/RL

L23 34808 L21/CAT

(L21 (L) CAT/RL)

=> s l21/catalyst

'CATALYST' IS NOT A VALID CROSSOVER QUALIFIER FOR L21

Answer sets created in a different file may be field qualified with a limited set of qualifiers. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> d his

(FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007)

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

L1 STRUCTURE UPLOADED

L2 7 S L1

L3 STRUCTURE UPLOADED

L4 6 S L3

L5 STRUCTURE UPLOADED

L6 4 S L5

L7 STRUCTURE UPLOADED

L8 0 S L7

L9 STRUCTURE UPLOADED

L10 0 S L9

L11 STRUCTURE UPLOADED

L12 2 S L11

L13 66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

L14 89 S L13

L15 57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

L16 STRUCTURE UPLOADED

L17 13 S L16

L18 338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

L19 455 S L18/RCT

L20 36 S L19 AND L15

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FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

E NICKEL/RN

E NICKEL/CN

L21 1 S E3

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007

L22 342935 S L21

L23 34808 S L21/CAT

=> s 122 and 123

L24 34808 L22 AND L23

=> s 122 and 120

L25 2 L22 AND L20

=> d 125, ibib abs hitstr, 1-2

L25 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:427623 HCAPLUS

DOCUMENT NUMBER: 141:7024

TITLE: A novel process for the preparation of  
2-aminomethylpyridine derivatives via Ni-catalyzed  
hydrogenation of 2-cyanopyridine derivatives

INVENTOR(S): Vangelisti, Manuel

PATENT ASSIGNEE(S): Bayer Cropscience Sa, Fr.

SOURCE: Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1422221	A1	20040526	EP 2002-356236	20021120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004046114	A1	20040603	WO 2003-EP14892	20031118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003290121	A1	20040615	AU 2003-290121	20031118
BR 2003014461	A	20050726	BR 2003-14461	20031118
EP 1565440	A1	20050824	EP 2003-782483	20031118
EP 1565440	B1	20061220		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1711244	A	20051221	CN 2003-80103328	20031118
JP 2006508143	T	20060309	JP 2004-552709	20031118
AT 348811	T	20070115	AT 2003-782483	20031118
US 2006004206	A1	20060105	US 2005-535723	20050520
PRIORITY APPLN. INFO.:			EP 2002-356236	A 20021120

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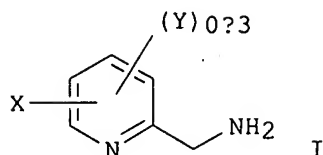
WO 2003-EP14892

W 20031118

OTHER SOURCE(S):

CASREACT 141:7024; MARPAT 141:7024

GI



AB The invention relates to a process for the preparation of 2-aminomethylpyridine derivs. of formula I [wherein: X is halogen atom; each Y may be the same or different and may be a halogen atom, a halogenoalkyl, an alkoxycarbonyl or an alkylsulfonyl], useful as intermediates for preparation of pesticides. 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine was prepared via Raney Ni-catalized hydrogenation of 2-cyano-3-chloro-5-trifluoromethylpyridine with a yield of 97%. The advantages of the proposed preparation of 2-aminomethylpyridine derivs. include the use of Raney nickel catalyst instead of expensive Pd catalyst (the Pd-catalyzed hydrogenation suffers from the disadvantage of dehalogenation reaction; Pd is also very sensitive to catalysts poisons).

IT 7440-02-0, Raney nickel, uses

RL: CAT (Catalyst use); USES (Uses)

(catalysts; novel process for the preparation of aminomethylpyridine derivs. via Raney Ni-catalyzed hydrogenation of cyanopyridine derivs.)

RN 7440-02-0 HCAPLUS

CN Nickel (CA INDEX NAME)

Ni

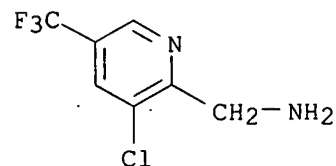
IT 175277-74-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(novel process for the preparation of aminomethylpyridine derivs. via Raney Ni-catalyzed hydrogenation of cyanopyridine derivs.)

RN 175277-74-4 HCAPLUS

CN 2-Pyridinemethanamine, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 80194-70-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; novel process for the preparation of aminomethylpyridine derivs.)

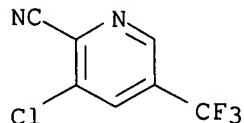
Updated Search

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via Raney Ni-catalized hydrogenation of cyanopyridine derivs.)

RN 80194-70-3 HCAPLUS

CN 2-Pyridinecarbonitrile, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:157737 HCAPLUS

DOCUMENT NUMBER: 136:200109

TITLE: Process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines.

INVENTOR(S): Dann, Norman; Riordan, Peter Dominic; Amin, Mehul Rasikchandra; Mellor, Michael

PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.

SOURCE: PCT Int. Appl., 18 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016322	A2	20020228	WO 2001-EP10984	20010821
WO 2002016322	A3	20020606		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1199305	A1	20020424	EP 2001-420128	20010607
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
CA 2415842	A1	20020228	CA 2001-2415842	20010821
AU 200213948	A	20020304	AU 2002-13948	20010821
EP 1311483	A2	20030521	EP 2001-982337	20010821
EP 1311483	B1	20061220		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2001013259	A	20030715	BR 2001-13259	20010821
JP 2004506716	T	20040304	JP 2002-521198	20010821
RU 2266900	C2	20051227	RU 2003-107931	20010821
CN 1721406	A	20060118	CN 2005-10088220	20010821
AT 348810	T	20070115	AT 2001-982337	20010821
EP 1746089	A1	20070124	EP 2006-120806	20010821

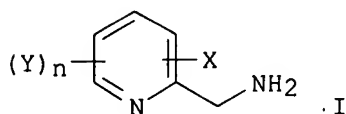
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R: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC,  
NL, PT, SE, TR

IN 2003MN00064	A	20050204	IN 2003-MN64	20030113
US 2004049048	A1	20040311	US 2003-362728	20030611
US 6921828	B2	20050726		
US 2005250947	A1	20051110	US 2005-177118	20050708
PRIORITY APPLN. INFO.:			GB 2000-21066	A 20000825
			GB 2000-25616	A 20001019
			EP 2001-420128	A 20010607
			CN 2001-814622	A3 20010821
			EP 2001-982337	A3 20010821
			WO 2001-EP10984	W 20010821
			US 2003-362728	A1 20030611

OTHER SOURCE(S): CASREACT 136:200109; MARPAT 136:200109  
GI



AB Title compds. (I; X = halo; Y = halo, haloalkyl, alkoxycarbonyl, alkylsulfonyl; n = 0-3) were prepared by catalytic hydrogenation of the corresponding 2-cyano derivs. Thus, 3-chloro-2-cyano-5-trifluoromethylpyridine (preparation given) was hydrogenated in MeOH over Pd/C containing HCl at 1 atmospheric to give 95-97% 2-aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride.

IT 7440-02-0, Nickel, uses  
RL: CAT (Catalyst use); USES (Uses)  
(process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines)

RN 7440-02-0 HCAPLUS

CN Nickel (CA INDEX NAME)

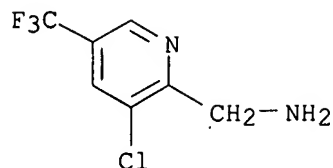
Ni

IT 326476-49-7P, 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines)

RN 326476-49-7 HCAPLUS

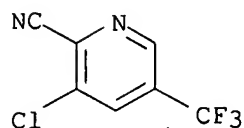
CN 2-Pyridinemethanamine, 3-chloro-5-(trifluoromethyl)-, hydrochloride (1:1) (CA INDEX NAME)

10535723



● HCl

IT 80194-70-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(process for preparation of 2-aminomethylpyridines by catalytic  
hydrogenation of 2-cyanopyridines)  
RN 80194-70-3 HCAPLUS  
CN 2-Pyridinecarbonitrile, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX  
NAME)



=> file caold  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
13.14	373.10

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.56	-1.56

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FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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more information.

=> d his

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FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

L1           STRUCTURE UPLOADED  
L2           7 S L1  
L3           STRUCTURE UPLOADED  
L4           6 S L3  
L5           STRUCTURE UPLOADED  
L6           4 S L5  
L7           STRUCTURE UPLOADED  
L8           0 S L7  
L9           STRUCTURE UPLOADED  
L10          0 S L9  
L11          STRUCTURE UPLOADED  
L12          2 S L11  
L13          66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

L14          89 S L13  
L15          57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

L16          STRUCTURE UPLOADED  
L17          13 S L16  
L18          338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

L19          455 S L18/RCT  
L20          36 S L19 AND L15

FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

            E NICKEL/RN  
            E NICKEL/CN  
L21          1 S E3

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007

L22          342935 S L21  
L23          34808 S L21/CAT  
L24          34808 S L22 AND L23  
L25          2 S L22 AND L20

FILE 'CAOLD' ENTERED AT 11:22:10 ON 06 JUL 2007

=> s l22 and l20

QUALIFICATION NOT VALID FOR L18

Field code qualifications can only be applied to text terms.

=> s l18 and l21

            10 L18  
            0 L21  
L26          0 L18 AND L21

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE           TOTAL

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	ENTRY	SESSION
FULL ESTIMATED COST	0.45	373.55
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	0.00	-1.56

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FILE CONTENT:1840 - 30 Jun 2007 VOL 147 ISS 2

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```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

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L27        STRUCTURE UPLOADED

=> s 127

SAMPLE SEARCH INITIATED 11:24:40 FILE 'CASREACT'  
SCREENING COMPLETE -        332 REACTIONS TO VERIFY FROM        49 DOCUMENTS

100.0% DONE        332 VERIFIED        1 HIT RXNS        1 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                              BATCH    \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS:        5548 TO        7732  
PROJECTED ANSWERS:                1 TO        79

L28        1 SEA SSS SAM L27 (        1 REACTIONS)

=> s 127 full

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 113.10 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 11:24:47 FILE 'CASREACT'  
SCREENING COMPLETE -        7961 REACTIONS TO VERIFY FROM        1065 DOCUMENTS

100.0% DONE        7961 VERIFIED        11 HIT RXNS        7 DOCS

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10535723

SEARCH TIME: 00.00.05

L29                7 SEA SSS FUL L27 (     11 REACTIONS)

=> d l29, ibib abs hitrxn, 1-7

'HITRXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
             must be entered on the same line as DISPLAY, e.g.,  
             D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
             all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
             hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format  
FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
             CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
             Summary for all hit reactions and fields containing  
             hit terms  
OCC ----- All hit fields and the number of occurrences of the  
             hit terms in each field. Includes total number of  
             HIT, PATH, SPATH reactions. Labels reactions that have  
             incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
             path". Displays all hit reactions, except those  
             whose steps are totally included within another hit  
             reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)

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RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short  
path". Displays all single step reactions which  
contain a hit substance. Also displays those  
multistep reactions that have a hit substance in both  
the first and last steps of the reaction, except for  
those hit reactions whose steps are totally included  
within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
codes. For a list of the display field codes, enter HELP DFIELDS  
at an arrow prompt (=>). Examples of combinations include: D TI;  
D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
be used with the DISPLAY command to display the record for a specified  
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):d his  
'D' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format

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10535723

FCRDREF ---- First hit in Compact Reaction Display (CRD) format with  
CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
Summary for all hit reactions and fields containing  
hit terms  
OCC ----- All hit fields and the number of occurrences of the  
hit terms in each field. Includes total number of  
HIT, PATH, SPATH reactions. Labels reactions that have  
incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
path". Displays all hit reactions, except those  
whose steps are totally included within another hit  
reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short  
path". Displays all single step reactions which  
contain a hit substance. Also displays those  
multistep reactions that have a hit substance in both  
the first and last steps of the reaction, except for  
those hit reactions whose steps are totally included  
within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
codes. For a list of the display field codes, enter HELP DFIELDS  
at an arrow prompt (=>). Examples of combinations include: D TI;  
D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
be used with the DISPLAY command to display the record for a specified  
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007)

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

L1               STRUCTURE UPLOADED  
L2               7 S L1  
L3               STRUCTURE UPLOADED  
L4               6 S L3  
L5               STRUCTURE UPLOADED  
L6               4 S L5  
L7               STRUCTURE UPLOADED  
L8               0 S L7  
L9               STRUCTURE UPLOADED  
L10              0 S L9  
L11              STRUCTURE UPLOADED  
L12              2 S L11  
L13              66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

L14              89 S L13

Updated Search

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L15 57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

L16 STRUCTURE UPLOADED

L17 13 S L16

L18 338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

L19 455 S L18/RCT

L20 36 S L19 AND L15

FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

E NICKEL/RN

E NICKEL/CN

L21 1 S E3

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007

L22 342935 S L21

L23 34808 S L21/CAT

L24 34808 S L22 AND L23

L25 2 S L22 AND L20

FILE 'CAOLD' ENTERED AT 11:22:10 ON 06 JUL 2007

L26 0 S L18 AND L21

FILE 'CASREACT' ENTERED AT 11:22:48 ON 06 JUL 2007

L27 STRUCTURE UPLOADED

L28 1 S L27

L29 7 S L27 FULL

=> d 129, ibib abs fhit, 1-7

L29 ANSWER 1 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:331318 CASREACT

TITLE: Biological evaluation of isothiazoloquinolones containing aromatic heterocycles at the 7-position: In vitro activity of a series of potent antibacterial agents that are effective against methicillin-resistant Staphylococcus aureus

AUTHOR(S): Wiles, Jason A.; Song, Yongsheng; Wang, Qiuping; Lucien, Edlaine; Hashimoto, Akihiro; Cheng, Jijun; Marlbor, Christopher W.; Ou, Yangsi; Podos, Steven D.; Thanassi, Jane A.; Thoma, Christy L.; Deshpande, Milind; Pucci, Michael J.; Bradbury, Barton J.

CORPORATE SOURCE: Achillion Pharmaceuticals, Inc., New Haven, CT, 06511-6653, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(5), 1277-1281

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

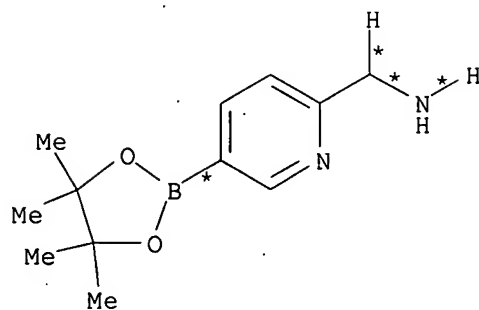
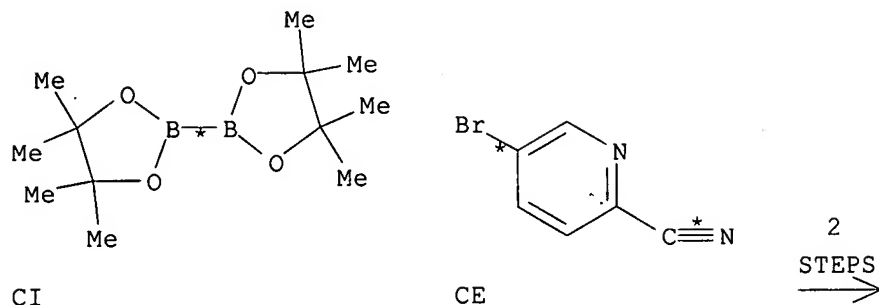
LANGUAGE: English

AB A diverse series of 9H-isothiazolo[5,4-b]quinoline-3,4-diones containing heteroarom. groups at the 7-position was prepared via palladium-catalyzed cross-coupling. Many of these compds. demonstrated potent antistaphylococcal activity (MICs  $\leq 2$   $\mu\text{g/mL}$ ) against a multi-drug-resistant strain (ATCC 700699) and low cytotoxic activity (CC50 > 100  $\mu\text{M}$ ) against the human cell line Hep2 (laryngeal carcinoma).

Updated Search

10535723

RX(46) OF 56 COMPOSED OF RX(40), RX(41)  
RX(46) CI + CE ==> AD



AD  
YIELD 100%

RX(40) RCT CI 73183-34-3, CE 97483-77-7  
RGT CK 127-08-2 AcOK  
PRO CJ 741709-63-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 67-68-5 DMSO  
CON 25 hours, 80 deg C

RX(41) RCT CJ 741709-63-7  
RGT CN 1333-74-0 H2  
PRO AD 880495-82-9  
CAT 7440-05-3 Pd  
SOL 64-19-7 AcOH  
CON 16 hours, room temperature

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

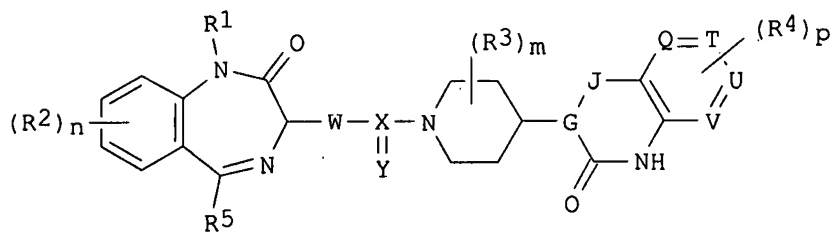
L29 ANSWER 2 OF 7 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 142:240471 CASREACT  
TITLE: Preparation of benzodiazepine derivatives as CGRP  
receptor antagonists

Updated Search

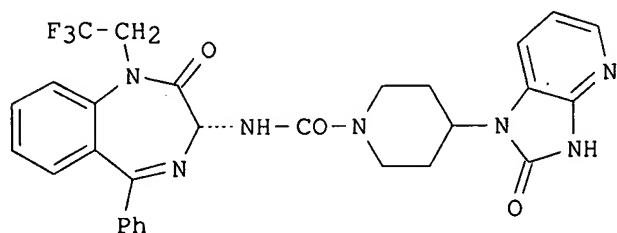
10535723

INVENTOR(S): Burgey, Christopher S.; Stump, Craig A.; Williams, Theresa M.  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: PCT Int. Appl., 79 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005013894	A2	20050217	WO 2004-US20209	20040624
WO 2005013894	A3	20060302		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004263080	A1	20050217	AU 2004-263080	20040624
CA 2529196	A1	20050217	CA 2004-2529196	20040624
EP 1641423	A2	20060405	EP 2004-776997	20040624
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1842526	A	20061004	CN 2004-80017996	20040624
JP 2007516183	T	20070621	JP 2006-517599	20040624
US 2006135511	A1	20060622	US 2005-562297	20051222
PRIORITY APPLN. INFO.:			US 2003-482854P	20030626
			WO 2004-US20209	20040624
OTHER SOURCE(S):			MARPAT 142:240471	
GI				



I

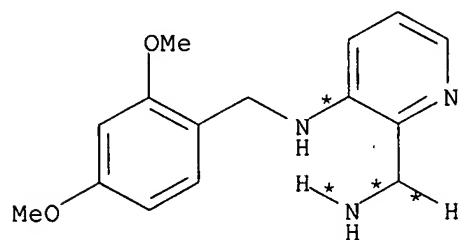
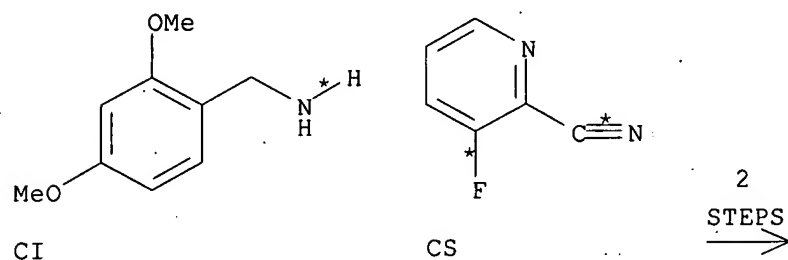


II



AB Benzodiazepine derivs. of formula I [R1 = H, alkyl, cycloalkyl, aryl, etc.; R2 = H, alkyl, cycloalkyl, aryl, etc.; R3 = H, alkyl, CO2H, alkoxycarbonyl; R4 = H, alkyl, cycloalkyl, aryl, etc.; R5 = H, alkyl, cycloalkyl, etc.; n = 1-4; m = 1-9; p = 1-4; W = O, (substituted) NH, (substituted) CH2; X = C, S; Y = O, NCONH2, etc.; G, J = N, NCH2, etc.; Q, T, U, V = CH, N; with provisos] are prepared as antagonists of CGRP receptors, and are useful in the treatment or prevention of diseases in which the CGRP is involved, such as headache, migraine and cluster headache. The invention is also directed to pharmaceutical compns. comprising these compds. and the use of these compds. and compns. in the prevention or treatment of such diseases in which CGRP is involved. Thus, II was prepared in several steps. The prepared compds. had IC50 values < 50  $\mu$ M against CGRP receptor.

RX(83) OF 165 COMPOSED OF RX(42), RX(43)  
 RX(83) CI + CS ==> CU



CU

RX(42) RCT CI 20781-20-8, CS 97509-75-6

STAGE(1)

RGT E 121-44-8 Et3N  
 SOL 127-19-5 AcNMe2  
 CON 4 hours, 80 deg C

STAGE(2)

RGT U 7732-18-5 Water

PRO CT 784155-72-2

RX(43) RCT CT 784155-72-2

10535723

STAGE(1)

RGT CN 16853-85-3 LiAlH4  
SOL 109-99-9 THF  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 0 deg C -> room temperature  
SUBSTAGE(3) 4 hours, room temperature

STAGE(2)

RGT CO 7757-82-6 Na2SO4  
SOL 7732-18-5 Water  
CON room temperature

PRO CU 784155-73-3

L29 ANSWER 3 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:123579 CASREACT

TITLE: Discovery and Evaluation of Potent P1 Aryl  
Heterocycle-Based Thrombin Inhibitors

AUTHOR(S): Young, Mary Beth; Barrow, James C.; Glass, Kristen L.;  
Lundell, George F.; Newton, Christina L.; Pellicore,  
Janetta M.; Rittle, Kenneth E.; Selnick, Harold G.;  
Stauffer, Kenneth J.; Vacca, Joseph P.; Williams,  
Peter D.; Bohn, Dennis; Clayton, Franklin C.; Cook,  
Jacquelynn J.; Krueger, Julie A.; Kuo, Lawrence C.;  
Lewis, S. Dale; Lucas, Bobby J.; McMasters, Daniel R.;  
Miller-Stein, Cynthia; Pietrak, Beth L.; Wallace,  
Audrey A.; White, Rebecca B.; Wong, Bradley; Yan,  
Youwei; Nantermet, Philippe G.

CORPORATE SOURCE: Medicinal Chemistry, Pharmacology, Biological  
Chemistry, Structural Biology, Molecular Systems and  
Drug Metabolism, Merck Research Laboratories, Merck  
and Co. Inc., West Point, PA, 19486, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(12),  
2995-3008

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

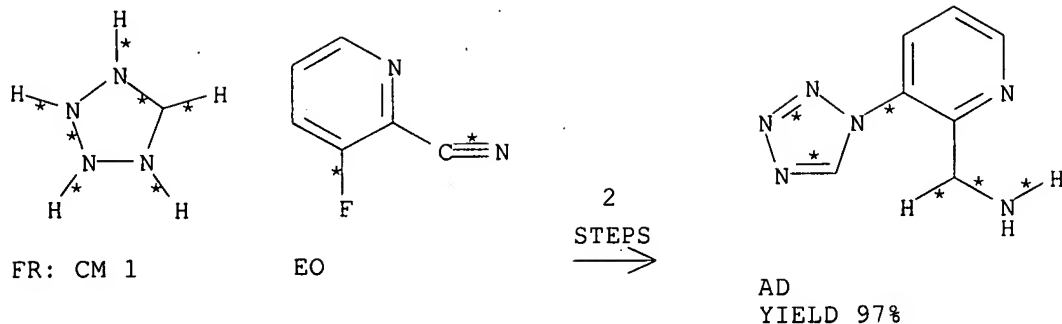
LANGUAGE: English

AB In an effort to discover potent, clin. useful thrombin inhibitors, a rapid  
analog synthetic approach was used to explore the P1 region. Various  
benzylamines were coupled to a pyridine/pyrazinone P2-P3 template. One  
compound, i.e. 2-[6-chloro-3-(2,2-difluoro-2-pyridin-2-yl-ethylamino)-2-oxo-  
2H-pyrazin-1-yl]-N-(2-[1,2,3]thiadiazol-4-yl-benzyl)acetamide, was found  
to have a thrombin Ki of 0.84 nM. A study of ortho-substituted  
five-membered-ring heterocycles was undertaken and subsequently  
demonstrated that the o-triazole and tetrazole rings were optimal.  
Combination of these potent P1 aryl heterocycles with a variety of P2-P3  
groups produced a compound with an extraordinary thrombin inhibitory  
activity of 1.4 pM. It is hoped that this potency enhancement in P1 will  
allow for more diversification in the P2-P3 region to ultimately address  
addnl. pharmacol. concerns.

RX(158) OF 284 COMPOSED OF RX(84), RX(85)

RX(158) FR + EO ==> AD

10535723



RX(84)      RCT    FR 27988-97-2

STAGE(1)

RGT    FT 2052-49-5 Bu4NOH  
SOL    7732-18-5 Water, 68-12-2 DMF

STAGE(2)

RCT    EO 97509-75-6  
CON    4 days, room temperature

PRO    FS 449758-32-1

RX(85)      RCT    FS 449758-32-1  
RGT    CR 1333-74-0 H2  
PRO    AD 449756-99-4  
CAT    7440-05-3 Pd  
SOL    64-17-5 EtOH  
CON    overnight, room temperature, 55 psi

REFERENCE COUNT:      22      THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 4 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:      141:7024 CASREACT

TITLE:      A novel process for the preparation of  
2-aminomethylpyridine derivatives via Ni-catalyzed  
hydrogenation of 2-cyanopyridine derivatives

INVENTOR(S):      Vangelisti, Manuel

PATENT ASSIGNEE(S):      Bayer Cropscience Sa, Fr.

SOURCE:      Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE:      Patent

LANGUAGE:      English

FAMILY ACC. NUM. COUNT:      1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1422221	A1	20040526	EP 2002-356236	20021120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004046114	A1	20040603	WO 2003-EP14892	20031118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				

Updated Search

10535723

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003290121 A1 20040615 AU 2003-290121 20031118  
 BR 2003014461 A 20050726 BR 2003-14461 20031118  
 EP 1565440 A1 20050824 EP 2003-782483 20031118  
 EP 1565440 B1 20061220

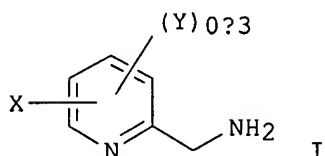
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

CN 1711244 A 20051221 CN 2003-80103328 20031118  
 JP 2006508143 T 20060309 JP 2004-552709 20031118  
 AT 348811 T 20070115 AT 2003-782483 20031118  
 US 2006004206 A1 20060105 US 2005-535723 20050520

PRIORITY APPLN. INFO.:

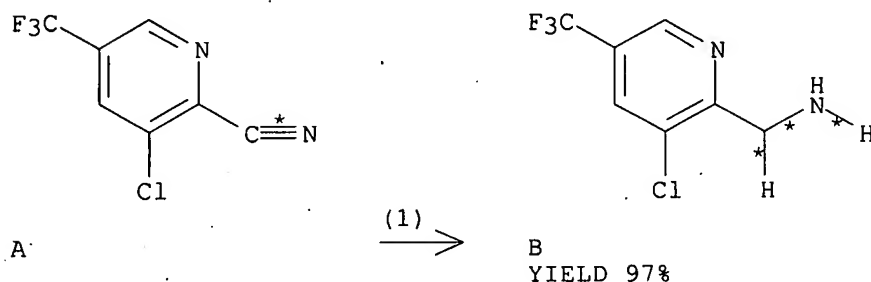
EP 2002-356236 20021120  
 WO 2003-EP14892 20031118

OTHER SOURCE(S): MARPAT 141:7024  
 GI



AB The invention relates to a process for the preparation of 2-aminomethylpyridine derivs. of formula I [wherein: X is halogen atom; each Y may be the same or different and may be a halogen atom, a halogenoalkyl, an alkoxy carbonyl or an alkylsulfonyl], useful as intermediates for preparation of pesticides. 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine was prepared via Raney Ni-catalyzed hydrogenation of 2-cyano-3-chloro-5-trifluoromethylpyridine with a yield of 97%. The advantages of the proposed preparation of 2-aminomethylpyridine derivs. include the use of Raney nickel catalyst instead of expensive Pd catalyst (the Pd-catalyzed hydrogenation suffers from the disadvantage of dehalogenation reaction; Pd is also very sensitive to catalysts poisons).

RX(1) OF 1 A ==> B



Updated Search

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RX(1) RCT A 80194-70-3  
RGT C 1333-74-0 H2  
PRO B 175277-74-4  
CAT 7440-02-0 Ni  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C, pH 7  
SUBSTAGE(2) 2 hours, 40 deg C, 18 bar, pH 7  
NTE Raney nickel used

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 5 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:272675 CASREACT

TITLE: Development of a Scaleable Synthesis of a  
3-Aminopyrazinone Acetamide Thrombin Inhibitor

AUTHOR(S): Ashwood, Michael S.; Alabaster, Ramon J.; Cottrell,  
Ian F.; Cowden, Cameron J.; Davies, Antony J.;  
Dolling, Ulf H.; Emerson, Khateeta M.; Gibb, Andrew  
D.; Hands, David; Wallace, Debra J.; Wilson, Robert D.  
CORPORATE SOURCE: Department of Process Research, Merck Sharp and Dohme  
Research Laboratories, Hoddesdon, Hertfordshire, EN11  
9BU, UK

SOURCE: Organic Process Research & Development (2004), 8(2),  
192-200

CODEN: OPRDFK; ISSN: 1083-6160

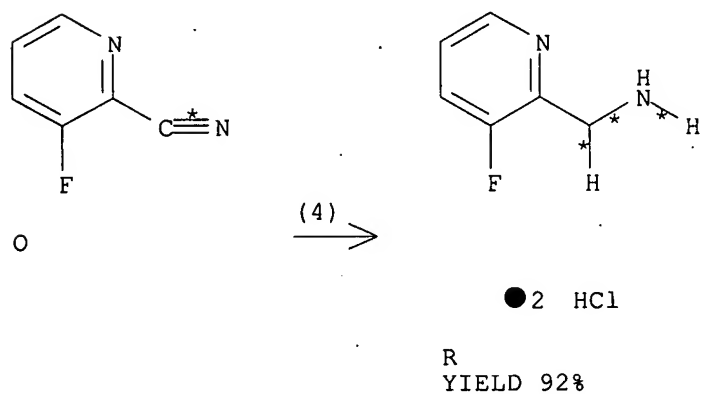
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A scaleable route to 2-{3-[(2,2-difluoro-2-(2-pyridyl)ethyl)amino]-6-chloro-2-oxohydropyrazinyl}-N-[(3-fluoro(2-pyridyl)methyl)acetamide (I) is described in which various scaleup issues were addressed to provide a safe, efficient, and robust route for the preparation of multi-kilo amts. of the compound. The use of expensive and toxic reagents, notably sodium azide, TMS-cyanide, and Deoxo-Fluor, and the need for specialist equipment were overcome in the preparation of the key fluorinated intermediates 2,2-difluoro-2-(2-pyridyl)ethylamine and 2-aminomethyl-3-fluoropyridine. With minimal isolations and through processing of intermediates, the thrombin inhibitor I was isolated in 36% overall yield.

RX(4) OF 84 ...O ==> R...



Updated Search

10535723

RX(4) RCT O 97509-75-6  
RGT S 7647-01-0 HCl, T 1333-74-0 H2  
PRO R 312904-49-7  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 18 hours, 20 deg C, 5 psi

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 6 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:198146 CASREACT

TITLE: Metabolism-Directed Optimization of 3-Aminopyrazinone  
Acetamide Thrombin Inhibitors. Development of an  
Orally Bioavailable Series Containing P1 and P3  
Pyridines

AUTHOR(S): Burgey, Christopher S.; Robinson, Kyle A.; Lyle, Terry  
A.; Sanderson, Philip E. J.; Lewis, S. Dale; Lucas,  
Bobby J.; Krueger, Julie A.; Singh, Rominder;  
Miller-Stein, Cynthia; White, Rebecca B.; Wong,  
Bradley; Lyle, Elizabeth A.; Williams, Peter D.;  
Coburn, Craig A.; Dorsey, Bruce D.; Barrow, James C.;  
Stranieri, Maria T.; Holahan, Marie A.; Sitko, Gary  
R.; Cook, Jacquelyn J.; McMasters, Daniel R.;  
McDonough, Colleen M.; Sanders, William M.; Wallace,  
Audrey A.; Clayton, Franklin C.; Bohn, Dennis;  
Leonard, Yvonne M.; Detwiler, Theodore J., Jr.; Lynch,  
Joseph J., Jr.; Yan, Youwei; Chen, Zhongguo; Kuo,  
Lawrence; Gardell, Stephen J.; Shafer, Jules A.;  
Vacca, Joseph P.

CORPORATE SOURCE: Departments of Medicinal Chemistry, Biological  
Chemistry, Drug Metabolism Molecular Systems,  
Structural Biology and Pharmacology, Merck Research  
Laboratories, West Point, PA, 19486, USA

SOURCE: Journal of Medicinal Chemistry (2003), 46(4), 461-473  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

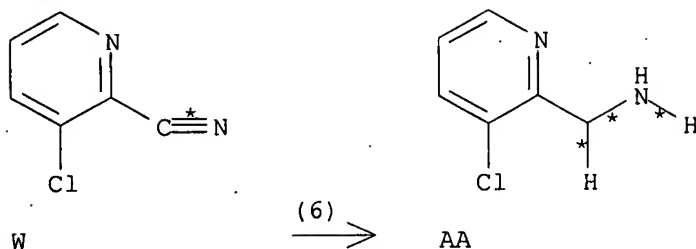
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Recent efforts in the field of thrombin inhibitor research have focused on  
the identification of compds. with good oral bioavailability and  
pharmacokinetics. In this manuscript we describe a metabolism-based approach  
to the optimization of the 3-(2-phenethylamino)-6-methylpyrazinone  
acetamide template which resulted in the modification of each of the three  
principal components (i.e., P1, P2, P3) comprising this series. As a  
result of these studies, several potent thrombin inhibitors were  
identified which exhibit high levels of oral bioavailability and long  
plasma half-lives.

RX(6) OF 261 ...W ==> AA...

10535723



RX(6) RCT W 38180-46-0  
 RGT AB 7664-41-7 NH<sub>3</sub>, AC 1333-74-0 H<sub>2</sub>  
 PRO AA 500305-98-6  
 CAT 7440-02-0 Ni  
 SOL 64-17-5 EtOH  
 CON 5 hours, 1 atm  
 NTE Raney nickel used

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 7 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:200109 CASREACT

TITLE: Process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines.

INVENTOR(S): Dann, Norman; Riordan, Peter Dominic; Amin, Mehul  
 Rasikchandra; Mellor, Michael

PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.

SOURCE: PCT Int. Appl., 18 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016322	A2	20020228	WO 2001-EP10984	20010821
WO 2002016322	A3	20020606		
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EP 1199305	A1	20020424	EP 2001-420128	20010607
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Updated Search

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RU 2266900	C2	20051227	RU 2003-107931	20010821
CN 1721406	A	20060118	CN 2005-10088220	20010821
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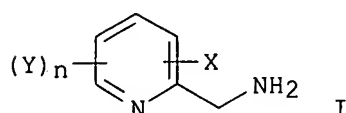
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US 2004049048	A1	20040311	US 2003-362728	20030611
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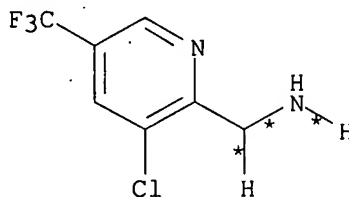
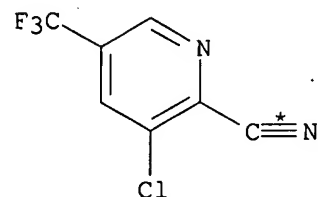
GB 2000-21066	20000825
GB 2000-25616	20001019
EP 2001-420128	20010607
CN 2001-814622	20010821
EP 2001-982337	20010821
WO 2001-EP10984	20010821
US 2003-362728	20030611

OTHER SOURCE(S): MARPAT 136:200109  
GI



AB Title compds. (I; X = halo; Y = halo, haloalkyl, alkoxycarbonyl, alkylsulfonyl; n = 0-3) were prepared by catalytic hydrogenation of the corresponding 2-cyano derivs. Thus, 3-chloro-2-cyano-5-trifluoromethylpyridine (preparation given) was hydrogenated in MeOH over Pd/C containing HCl at 1 atmospheric to give 95-97% 2-aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride.

RX(1) OF 1 A ==> B



● HCl

YIELD 97%

RX(1) RCT A 80194-70-3  
RGT C 1333-74-0 H2, D 7647-01-0 HCl

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10535723

PRO B 326476-49-7  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH

Updated Search